

Electronic transmission in bent quantum wires

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Electronic transmission in bent quantum wires modeled by the tight binding Hamiltonian, and clamped between ideal, semi-infinite leads is studied. The effect of ‘bending’ the chain is simulated by introducing a non-zero hopping between the extremities of the wire. It is seen that the proximity of the two ends gives rise to Fano line shapes in the transmission spectrum. Transmission properties for both an ordered lattice and a Fibonacci quantum wire are discussed. In the quasi-periodic Fibonacci chain, the proximity of the two ends of the chain closes all the gaps in the spectrum and the spectrum loses its Cantor set character.

PACS numbers: 64.60.aq, 63.22.-m, 73.63.Nm, 71.23.An

I. INTRODUCTION

Winding chains as models of conducting polymers present several interesting features in their electronic spectrum and transport properties [1, 2]. As a result of winding at one or more places in the chain an electron gets an alternative path to hop to a site, which might have been a distant neighbor otherwise. This *short cut* path provided to the propagating electron leads to non-trivial transport characteristics, sometimes leading to groups of states with very large localization length, indicative of a metal-insulator transition [1]. The features persist and become even richer when more than one chains couple in the transverse direction with random winding structure [2]. It has recently been argued that such simple models of the conducting polymers where an electron travels along a randomly tangled chain has the geometry of a “small-world network” [3], and may lead to a multifractal set of single particle states.

There is another aspect of interest hidden in such simple models that are quite relevant in the context of the present development of mesoscopic physics or of nanotechnology. It is now possible to build up ‘atomic chains’ using the scanning tunneling microscope (STM) tip as tweezers. The tailor made quantum devices in recent years have inspired immense research on quantum wires (QW) and quantum dots (QD) that have been major areas in nano-electronics and nano structure physics [4, 5]. Electronic transport in an array of QD’s or in a QW can now be studied in a controllable way [6, 7], and a wide variety of theoretical studies based on simple orbital [8]-[10] tight binding models have been reported in the literature that reproduce several basic features of quantum transport in QD arrays, QW or molecular wires [11].

In this communication we present a blend of the spirits of the studies of electronic transport in winding polymers and the model studies on QW systems within a single orbital tight binding scheme. Our interest is divide into two parts. First, We address the changes observed in the spectrum and transport characteristics of a QW modeled by an array of atomic sites, when the ‘wire’ is bent so as to provide the traveling electron with an additional, *short cut* path to jump over to an otherwise distant site

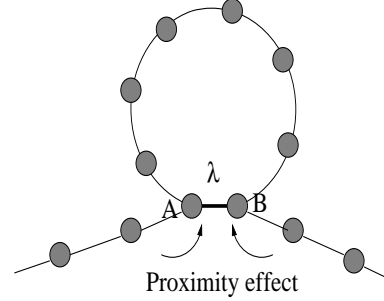


FIG. 1: A one dimensional ordered quantum wire is bent to bring two ‘end atoms’ close enough to ensure a tunnel effect. λ is the tunnel hopping integral.

in the chain. The ‘closeness’ between two sites in the chain, brought about by the ‘bending’, will be modeled by an additional hopping amplitude along the shortcut path, and it’s effect on the transmission spectrum will be discussed.

Second, we examine the transmission spectrum of a quasi-periodic Fibonacci chain, bent and clamped between two semi-infinite ordered leads. Usually, a Fibonacci quasi-periodic chain, in the thermodynamic limit, exhibits a completely multifractal Cantor set spectrum [12, 13, 14, 15]. The fragmented character of the spectrum is reflected in a transport calculation of such chains clamped between the leads. We wish to investigate the effect of the short cut path generated as a result of bending the chain on the single particle transport in a Fibonacci chain of arbitrarily large size. This might throw light on the basic question of conductance of an aperiodic QW, or arrays of QD’s when their geometry is deformed in some way so as to allow for any tunneling effect within the wire.

Our results are quite interesting. In the ordered lattice we find the creation of states localized at the points of bending and sharp asymmetric Fano like line shapes [16, 17, 18] in the transmission, a simple case of which is worked out analytically here. The fragmented Cantor spectrum of a Fibonacci chain is found to be grossly affected by the bending, and all the gaps close with the onset of the hopping across the short cut path.

The results, to the best of our knowledge, throw light on some of the basic facts that have not been discussed in details elsewhere.

In what follows we describe the results. In section I we present the model and the density of states of a bent ordered chain. Section II deals with the transmission spectrum of the bent ordered chain with an analysis of the Fano line shape in the simplest case. Section III deals with the quasi-periodic Fibonacci chain bent and clamped between two semi-infinite leads, and its transport properties, and we draw conclusion in section IV.

II. THE MODEL AND THE ENERGY SPECTRUM: THE PERIODIC CASE

We adopt a tight binding formalism, and incorporate only the nearest neighbor hopping. We begin by referring to Fig. 1. We deal with non-interacting electrons and the single band Hamiltonian is given by,

$$H = \sum_i \epsilon_i c_i^\dagger c_i + \sum_{\langle ij \rangle} t_{ij} (c_i^\dagger c_j + c_j^\dagger c_i) \quad (1)$$

where, c_i (c_i^\dagger) are the annihilation (creation) operator at the i th site of the chain, ϵ_i is the on-site potential at the i -th site which we shall choose as ϵ_0 for each site when the chain is periodic. t_{ij} is the nearest neighbor hopping integral, that will be taken as t in the bulk portion of an ordered chain, and will be equal to λ for hopping from the site A to B and vice versa.

To obtain the local density of states (LDOS) at the junctions A and B of the bent system we make use of the system of equations satisfied by the Green's function G_{ij} , viz,

$$(E - \epsilon_i)G_{ij} = \delta_{ij} + \sum_k t_{ik}G_{kj} \quad (2)$$

On the right hand side of Eq. 2 the index k runs over the nearest neighbors of the i -th site. Obviously, t_{ik} is equal to t or, λ as the case may be. To evaluate the LDOS at the site A (or, B) we first re-normalize the portion of the chain 'trapped' between the vertices A and B into an effective *diatomic molecule* AB . The effective on-site potential at the site A is given by,

$$\tilde{\epsilon}_A = \epsilon_0 + t \frac{M_{12}}{M_{11}} \quad (3)$$

Naturally, $\tilde{\epsilon}_B = \tilde{\epsilon}_A$. The re-normalize hopping integral connecting the A site with the B site (when the intermediate sites are decimated [19]) is given by,

$$t_{AB} = \lambda + \frac{t}{M_{11}} \quad (4)$$

Here, λ represents the short circuit hopping that results out of the bending of the wire, $M_{11} = U_N(x)$, and $M_{12} = -U_{N-1}(x)$ with $U_N(x)$ being the N th order Chebyshev

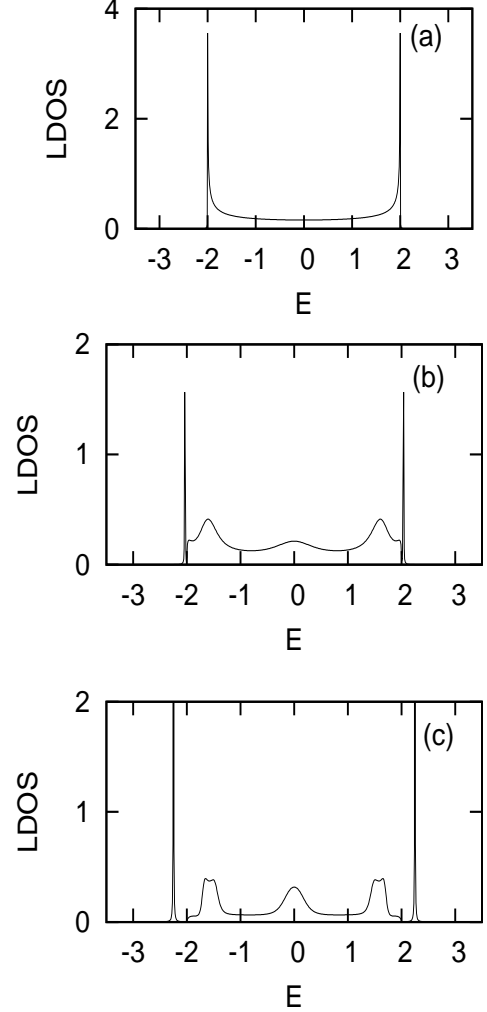


FIG. 2: Local density of states at the A (or, B) site without and with bending. The figures correspond to (a) a purely linear chain with no bending, i.e. $\lambda = 0$ (dashed line), (b) $\lambda = 0.6$ and (c) $\lambda = 1.0$ when the wire bends. Figures (b) and (c) refer to the situation when $N = 6$. We have chosen $\epsilon_0 = 0$ and $t = 1$ and E and λ are measured in unit of t .

polynomial of the second kind, and $x = (E - \epsilon_0)/2t$. E is the energy of the electron, and N represents the number of atoms trapped in the bent portion of the chain in between the vertices A and B .

The LDOS at the site A (or, equivalently, at B) is then easily obtained by a well known decimation renormalization group (RG) method discussed elsewhere [19]. In Fig.2 we show the LDOS at the site A (or, B) when the chain is not folded (Fig.2a), and folded with increasing values of the short circuit hopping λ (Fig.2b and 2c). While, in the first case, as expected, we get back the standard LDOS profile for a periodic chain, in the two latter cases the growth of two localized levels right beyond the values $E = \pm 2$ is apparent. As the short circuit hopping λ increases, the localized levels move away from

the band edges of the perfectly periodic open chain. The states are strictly localized at the edges A and B . It is also interesting to note that apart from generating a couple of localized levels, a non-zero value of the cross hopping λ changes the profile of the LDOS in a non-trivial fashion. In particular, the center of the band exhibits an oscillation in the values of the LDOS compared to the relatively flat low value in the case of an open chain, as λ increases. This feature can be taken to be a consequence of the proximity of the sites A and B .

III. TRANSMISSION CHARACTERISTICS

We now address the transmission properties of a bent quantum wire modeled by the sites sitting in a peri-

odic array and folded at the two points A and B as shown in Fig.1. To calculate the transmission coefficient we consider the folded portion of the infinite system as our ‘sample’ and the remaining portions of the chain extending from the vertices A and B to infinity on either side as two semi-infinite ordered leads. The bent part of the system trapped between the vertices A and B is re-normalized [19], and we arrive at an effective diatomic molecule $A-B$ clamped between the leads. The effective on-site potentials at the sites $A(B)$ are given by Eq.(3) and the effective hopping between the atoms \tilde{A} and \tilde{B} is given by t_{AB} as we have already worked out. The transmission coefficient is given by the well known formula [20],

$$T = \frac{4 \sin^2 ka}{[M_{12} - M_{21} + (M_{11} + M_{22}) \cos ka]^2 + (M_{11} + M_{22})^2 \sin^2 ka} \quad (5)$$

where, $M_{11} = U_N(x)$, and $M_{12} = -M_{21} = -U_{N-1}(x)$, and $M_{22} = -U_{N-2}(x)$. $U_N(x)$ is the N th order Chebyshev polynomial of the second kind, $x = (E - \epsilon_0)/2t$, and $ka = \cos^{-1}[(E - \epsilon_0)/2t]$. The lattice spacing a of the chain is taken to be unity in all results presented here. Before presenting any general result we draw the attention of the reader to a special feature of the transmission profile, viz, the appearance of the Fano line shape [16, 18].

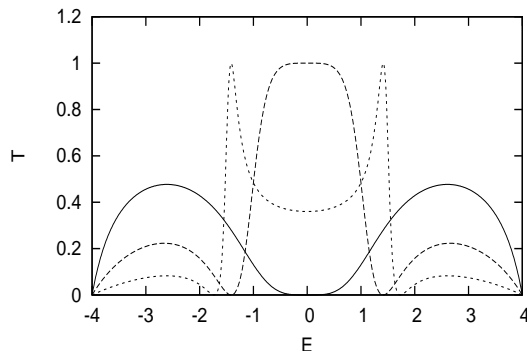


FIG. 3: Transmission across a bent ordered chain with $N = 2$ when $\lambda = 2$ (solid line), $\lambda = 4$ (dashed line) and $\lambda = 8$ (dotted line). We have taken $\epsilon_0 = 0$ and $t = 1$, and λ is measured in unit of t .

To get a clear understanding, we work out the very simple case of bending when there is just one atom in the arc between the junctions A , and B . That is, we take $N = 1$. In this case, the on-site potentials at the end atoms, and the effective hopping t_{AB} of the ‘diatomic

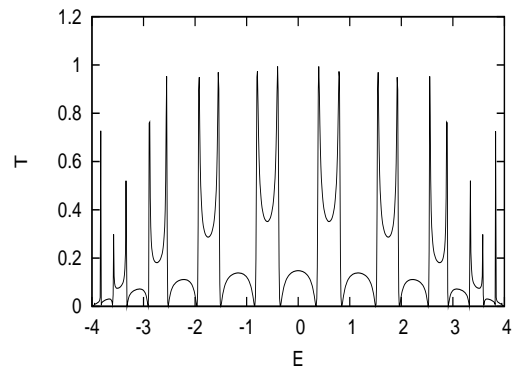


FIG. 4: Transmission across an bent ordered chain of 22 atoms with $\lambda = 8$. Asymmetric Fano line shape appears at every anti-resonance point. Other parameters are the same as in Fig.4

molecule’ clamped between the leads are given by,

$$\begin{aligned} \tilde{\epsilon}_A &= \epsilon_0 + \frac{t^2}{E - \epsilon_0} \\ t_{AB} &= \lambda + \frac{t^2}{E - \epsilon_0} \end{aligned} \quad (6)$$

Clearly, an anti-resonance will occur at

$$E = \epsilon_0 - \frac{t^2}{\lambda} \quad (7)$$

Evidently, as $\lambda \rightarrow \infty$ (atomic sites A and B coming indefinitely close together), the anti-resonance shifts towards the center of the spectrum, i.e. towards $E = \epsilon_0$.

It is quite straightforward (at the expense of a little algebra though) to show that as $\lambda \rightarrow \infty$, then in a δ -neighborhood of the anti-resonance, i.e., for $E = \epsilon - t^2/\lambda + \delta$, such that the product $\lambda\delta$ remains finite, the transmission amplitude τ ($T = |\tau|^2$) can be approximately written as,

$$\tau = e^{i\pi} \frac{4t}{\lambda} \left[\frac{\delta}{(\delta + \frac{t^2}{\lambda}) - i \frac{2t^3}{\lambda^2}} \right] \quad (8)$$

The term within the square bracket controls the line shape of the transmission characteristic around the point of anti-resonance while the pre-factor $4t/\lambda$ gives the amplitude. Two points are to be noted. First, as λ increases, the amplitude of transmission drops. Second, The numerator inside the square bracket is simply δ , which will be zero as $\delta \rightarrow 0$, while the real part of the denominator in the square bracketed term has a zero at $\delta = -t^2/\lambda$. These de-tuned zeros give rise to an asymmetric Fano line shape around the point of anti-resonance as is already discussed in the literature [18, 21]. The width of the transmission profile is of course, given by the remaining term $2t^3/\lambda^2$.

For $N > 1$, the analytical attack to reveal any Fano profile, though not impossible, becomes a bit complicated, and a straightforward use of Eq. (5) is advised for the numerical evaluation of the transmission coefficient. Fig.3 displays the features for $N = 2$ with $\lambda = 2t$ (solid line), $4t$ (dashed line) and $8t$ (dotted line) respectively. For $\lambda = 2t$, the transmission is low in general (compared to an open periodic chain, and hinting to the fact that the proximity effect induces some destructive interference), with a broad minimum around the center of the spectrum. As λ grows the spectrum is marked by the appearance of a couple of transmission resonance peaks for $\lambda = 4t$, which merge into a broad maximum when $\lambda = 8t$. The development of asymmetric Fano profile around the $T = 0$ points is obviously on the cards, and becomes much more prominent as we increase N , the number of atoms trapped in the bent portion (Fig.4).

IV. TRANSMISSION IN A BENT FIBONACCI WIRE

We now present results for a bent quasi-periodic Fibonacci chain clamped between two semi-infinite leads in such a manner that the lead-sample connecting points are close enough to ensure a tunnel-hopping across the junctions (Fig.5).

The Fibonacci chain is the canonical example of quasi-periodic order in one dimension. The eigenvalue spectrum is known to be a Cantor set with measure zero [12]. The chain is grown recursively using two symbols L and S that stand for bonds with two different hopping strengths, viz, t_L and t_S in our case. The growth rule is, $L \rightarrow LS$ and $S \rightarrow L$, with the first generation chain comprising of a single L -bond. In the corresponding tight

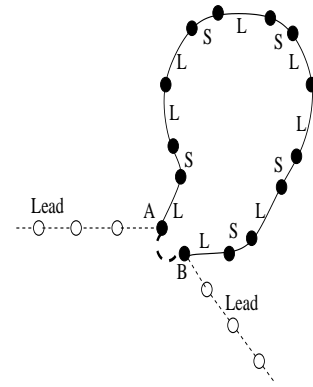


FIG. 5: A quasi-periodic Fibonacci chain (transfer model) is bent to bring the ‘end atoms’ in close proximity. The *short cut* hopping is shown as the dotted line connecting A and B.

binding Hamiltonian, the on-site potentials assume three possible values depending on the nearest neighbor configuration of any vertex, viz, ϵ_α , ϵ_β and ϵ_γ when an atomic site is flanked by the bonds $L-L$, $L-S$ and $S-L$ on its two sides respectively.

Without losing any generality, we consider odd generation chains clamped between the ordered leads. The trapped portion of the chain is then re-normalized using the recursion relations,

$$\begin{aligned} \epsilon_\alpha(n+1) &= \epsilon_\alpha(n) + \frac{t_L(n)^2(2E - \epsilon_\beta(n) - \epsilon_\gamma(n))}{\delta(n)} \\ \epsilon_\beta(n+1) &= \epsilon_\alpha(n) + \frac{t_L(n)^2(E - \epsilon_\beta(n))}{\delta} + \frac{t_L(n)^2}{E - \epsilon_\beta(n)} \\ \epsilon_\gamma(n+1) &= \epsilon_\gamma(n) + \frac{t_L(n)^2(E - \epsilon_\gamma(n))}{\delta} + \frac{t_S(n)^2}{E - \epsilon_\beta(n)} \\ t_L(n+1) &= \frac{t_L(n)^2 t_S(n)}{\delta(n)} \\ t_S(n+1) &= \frac{t_L(n) t_S(n)}{E - \epsilon_\beta(n)} \end{aligned} \quad (9)$$

where, $\delta(n) = (E - \epsilon_\beta(n))(E - \epsilon_\gamma(n)) - t_S(n)^2$.

As in the previous section, the transmission coefficient is obtained after decimating [18] all the sites of the Fibonacci chain trapped in the bent portion thereby creating an effective diatomic molecule as before. Fig. 6 shows the transmission spectrum for the set of values $\epsilon_\alpha = \epsilon_\beta = \epsilon_\gamma = 0$, $t_L = 1 = t_S/2$ and $\lambda = 8$. It is interesting to observe that all the gaps which are present in an open Fibonacci chain are absent in the presence of the short cut hopping λ .

Asymmetric Fano line shape is now found to be associated with every anti-resonance in the transmission spectrum. Fig.6b displays the magnified version of the $T-E$ graph between $E = \pm 1$ (E is measured in unit of t_L which we select as unity). It is interesting to observe that the figure indeed displays the characteristic

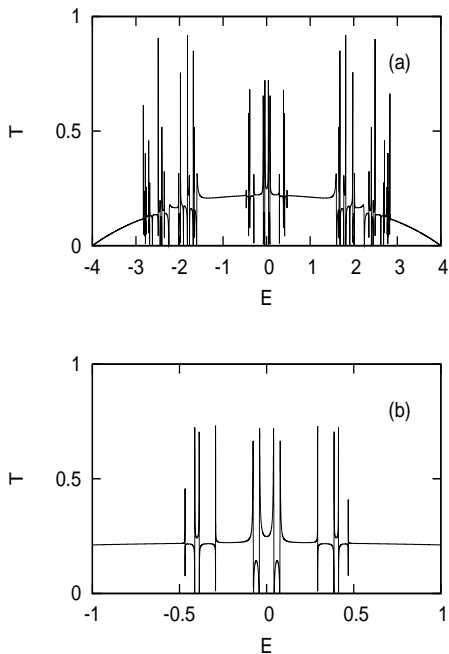


FIG. 6: Transmission across a 9-th generation Fibonacci chain with proximity effect. $\lambda = 8$, $\epsilon_\alpha = \epsilon_\beta = \epsilon_\gamma = 0$, $t_L = 1$ and $t_S = 2$.

self-similarity of the spectrum of a quasi-periodic open chain, but now every gap that is found in the spectrum of an open Fibonacci chain is found to be closed. This is the effect of the proximity of the two extreme points A and B in the lattice. The Fano line shape becomes much more prominent.

Though, we have shown in Fig.6 the transmission spectrum for a somewhat bigger value of the cross hopping λ , extensive numerical investigation reveals that the closing

of the gaps, at every scale of the energy, happens whenever the tunneling of the electron is allowed between the contact points directly, i.e., even with a very small value of λ . This opens up a question regarding the stability of the cantor set eigenvalue spectrum in a realistic Fibonacci quantum wire that is bent so as to bring its two ends to close proximity.

V. CONCLUSION

In conclusion, we have addressed the question of two terminal transmission across a linear chain when a portion of it is bent so as to bring two distant atomic sites into close proximity. An ordered chain and a quasi-periodic chain are discussed. For the ordered case it is shown that, the bending and the corresponding cross hopping of electrons generates Fano line shape in the transmission profile, a simple example of which is analytically examined. The overall transmittance is reduced as the cross hopping is switched on, and some resonance peaks mark the spectrum. Localized states are created with a non-trivial change in the central part of the energy spectrum. For the quasi-periodic chain, the bending destroys the gaps in the spectrum at all scales of energy. The self-similar character is somewhat retained, and Fano like line shapes are likely to mark every transmission anti-resonance. On finer scan of the energy interval, the closing of the gaps becomes more and more apparent.

ACKNOWLEDGMENT

Illuminating conversations with Rudolf A. Römer, Alberto Rodriguez, and Santanu Maiti are gratefully acknowledged.

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